

Dynamical Coarse Graining of Large Scale-Free Boolean networks

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We present a renormalization-grouplike method performed in the state space for detecting the dynamical behaviors of large scale-free Boolean networks, especially for the chaotic regime as well as the edge of chaos. Numerical simulations with different coarse-graining level show that the state space networks of scale-free Boolean networks follow universal power-law distributions of in and out strength, in and out degree, as well as weight. These interesting results indicate scale-free Boolean networks still possess self-organized mechanism near the edge of chaos in the chaotic regime. The number of state nodes as a function of biased parameter for distinct coarse-graining level also demonstrates that the power-law behaviors are not the artifact of coarse-graining procedure. Our work may also shed some light on the investigation of brain dynamics.

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Boolean networks are considered to be an important approach for characterizing the dynamics of complex systems consisting of interacting units. Examples of such systems cover as diverse as social and economic networks, neural networks, protein protein interaction networks and regulatory networks. Random Boolean network, a very simple and general model, since introduced by Kauffman in 1969 [2, 3], has drawn much attention from not only social and biological communities but also physical community. Intensive investigations indicate that abundant dynamical properties exist in the random Boolean networks, classified to ordered and chaotic behaviors [4]. However, in recent years, more and more empirical evidences demonstrate that scale-free (SF) structural properties are ubiquitous in nature [5, 6]. Therefore, collective Boolean dynamics on SF networks have been studied for revealing the effect of structural properties on the dynamics [7]. Dynamics in the ordered regime of both random and SF networks are fully explored and attractive cycles (or called attractors) are found, which is attributed to the self-organized mechanism. However, due to the restriction of computing ability and the complexity of the critical dynamical behaviors, a thorough description of the dynamics in the chaotic regime as well as the edge of chaos, especially for large networks, remains unclear.

A Boolean network is composed of interacting units (nodes) x_1, \dots, x_n . The state of each unit $\sigma(x_i) \in 0, 1 (i = 1, \dots, N)$ is a binary variable. The next time state of any given unit is determined by both its input from other units or itself and its assigned Boolean function F_i . All the states of units are allowed to update synchronously. At each time step, the state of the Boolean network $S(t)$ is denoted by all the N units together: $S(t) = (\sigma(x_1(t)) \ \sigma(x_2(t)) \ \dots \ \sigma(x_N(t)))$. Thus the state space consists of all the possible states of the Boolean network. For example, if $N = 10000$, the state space has 2^{10000} different states. Each distinct state $S(t)$

is represented by a node in the state space and directed links exist between $S(t)$ and $S(t+1)$ with direction from $S(t)$ to $S(t+1)$. Then the evolution of a Boolean system can be characterized by a state graph. When the Boolean system is in the ordered regime, it has been proved that no matter what the initial state of the system is, the state graph will rapidly converge to a very small periodic cycle. This behavior is explained as the “origin of order” of complex systems. However, as to the chaotic state as well as the edge of chaos, no one knows the specific state graph in the state space unless for very small network size.

In this letter, we present a coarse-graining method to detect the structure of state graph of SF Boolean networks. Our method is partially inspired by Kim [8], who proposes a geographic coarse graining process for detecting the structural properties of networks of huge size. We first place the Boolean units on the nodes of a geographical embedded SF network (or called SF network on lattices) following Ref. [9]. The network is established as follows: $N = L \times L$ nodes are put on lattice's points of the two dimensional square net, whereafter the degree k of each node is chosen according to a given degree distribution function $P(k) \sim k^{-\alpha}$. Here, we fix $\alpha = 3$ for simplicity. A node i is selected at random and then its assigned links (the number is k_i) are realized on the basis that the geographically closer vertices are connected first. Then repeat this procedure until all the nodes are dealt with. As a remark, this connecting process will lead to a cut off of degree distribution beyond which $P(k)$ follows a power-law form $P(k) \sim k^{-\gamma}$. Without losing generality, we also assume links are bidirectional and each pair of nodes on both sides of each given link is the input for each other.

After constructing the network structure, we assign each unit (node) $i = 1, \dots, N$ a Boolean function F_i according to two “effective” inputs, that is, the state of the unit itself and the average state of all its neighbors

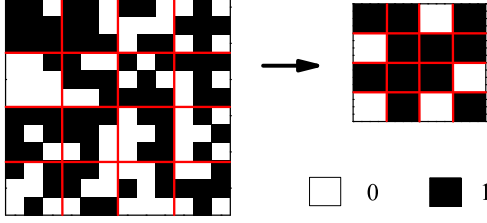


FIG. 1: An example of coarse-graining procedure. The color coding is that white represents a node with state 0 and black a node with state 1. The original network in the right side is divided into 4×4 identical size boxes with 3×3 nodes counted to each box. If the nodes with state 1 in a box take the majority, the box's state is 1; otherwise it is 0. Then the system's state is represented by the coarse-grained graph and the state space is composed of $2^{4 \times 4}$ different states.

[10]. The latter is a majority rule. The input of each unit from its neighbors is determined by the majority of the neighbors; that is if the majority's state is 1, then the input will be 1; if the number of units with state 1 is equal to that with state 0 among its neighbors, the input will be ξ ; otherwise 0 is inputted. Therefore, the number of selectable Boolean functions of each unit is $2^{2 \times 3} = 64$ [10]. The advantage of this assignment is that the number of the units' input is independent of their connectivity, which produces certain correspondence to the classical random Boolean networks. Hence, we can discuss the effect of the number of input and the biased parameter P compared with the existent results. Here, P is the probability of choosing functions with an outcome 0 and correspondingly with probability $1 - P$ for the functions with an outcome 1 [7]. For example, $P = 1$ means the outcome of the chosen function for any given input is always 0; $P = 0$ indicates the output must be 1. Refer to the Random Boolean networks, the edge between ordered and chaotic state is described by a function $2P(1 - P) = 1$, where K is the average input number of the units and P is the biased parameter. The case $P = 0.5$, $K = 2$ is at the boundary and in this condition the Boolean function space is composed of $2^{2^K} = 16$ different selectable functions. As to our assignment, the space is composed of $64 \simeq 2^{2^{2.6}}$ functions, which indicates that the SF Boolean network is in the chaotic regime and near the edge of chaos [4]. Below, we will provide further evidences for this conclusion.

So far we have given the network structure and the unit evolutionary rule controlled by the Boolean function, the Boolean network can evolve step by step and a directed state network is formed. Unfortunately, when the system is in the chaotic regime, the network is so huge that no super computers can support it. Hence, we

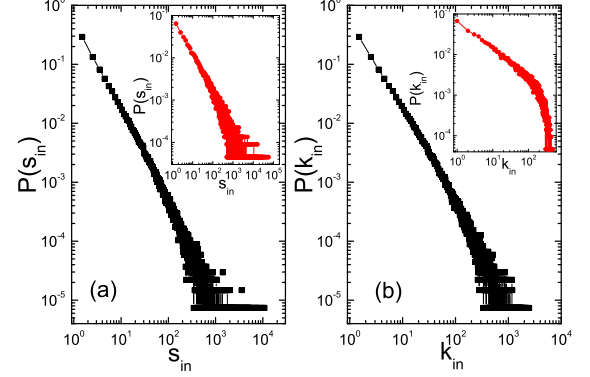


FIG. 2: (a) In-strength and (b) in-degree distributions of the coarse-grained state network using 4×4 boxes with $N = 100 \times 100$ Boolean nodes. The insets of (a) and (b) are the in-strength and in-degree of coarse-grained state network using 3×3 boxes with $N = 99 \times 99$ nodes, respectively.

present a coarse-graining procedure which groups a large quantities of state nodes at the state space to a single one. This procedure is described as follows: As shown in Fig. (1), at each time step, after each unit updates its state, we divide the units on the square lattice into $m \times m$ square boxes with identical size. Each box is considered as a new node whose state at this step is determined by a majority rule; that is, if the units with state 1 in a box take the majority, then the state of the box is 1; Otherwise, the box's state is 0. Therefore the huge state space of the SF Boolean network is reduced to $2^{m \times m}$ and the computation ability allows to record every state and depict the shrank networks in the state space. Note that this coarse-graining procedure does not affect the evolution of the Boolean units, but just unbiased shrinks large amount of state together. Moreover, the statistic properties of the original state graph can be reflected by the coarse-grained one, which will be demonstrated later.

The structural properties of the coarse-grained state networks can be quantified by the distributions of degree, strength as well as weight. As mentioned early, the state networks are directed with each node pointing to the next time state node. Then the basic structural properties of directed networks including in-degree and out-degree can be naturally introduced here to characterize the structural properties of the networks. In-degree of a given node denotes the number of its neighbors with directed connections pointing to it. In parallel, out-degree of a node represents the directed links going out from it. However, the state networks are far from pure topological structures which will miss important statistic features. Suppose that a state node arrives at another node more than one time, this information will be neglected by the description of node degree. This thus calls for

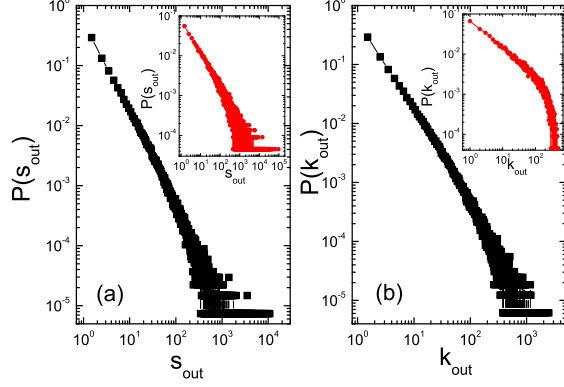


FIG. 3: (a) In-strength and (b) in-degree distributions of the coarse-grained state network using 4×4 boxes with $N = 100 \times 100$ Boolean nodes. The insets of (a) and (b) are results of more heavily coarse-grained state networks with adopting 3×3 boxes, the original Boolean network size is $N = 99 \times 99$.

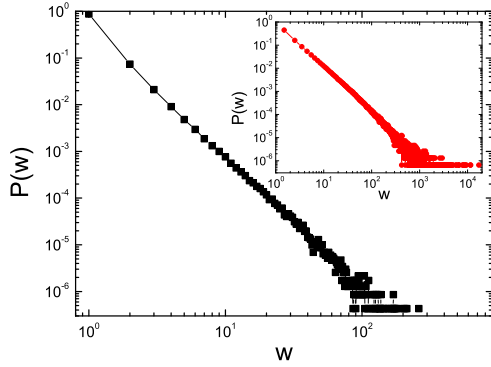


FIG. 4: Weight distribution by adopting 4×4 boxes and 3×3 boxes (the inset) with original Boolean network size $N = 100 \times 100$ and 99×99 , respectively.

the use of weighted adjacency matrix element $w_{i \rightarrow j}$ representing the times the state trajectory going from node i immediately to node j . A natural generalization of degree in the case of weighted networks is the node strength (strength for short). The strength is also divided into in-strength and out-strength, respectively. The in-strength is defined as $s_{in}^i = \sum_{j \in \Gamma} w_{j \rightarrow i}$, correspondingly, the out-strength $s_{out}^i = \sum_{j \in \Gamma} w_{i \rightarrow j}$, where the sum runs over the neighbor set $\Gamma(i)$ of node i .

We now focus on the statistic structural features of the state networks in terms of the distributions of strength, degree and weight. We start the simulations from a SF network on lattice with degree distribution following a power law $P(k) \sim k^{-3}$. Initial state of each Boolean unit (node) is assigned randomly. Then each node updates its

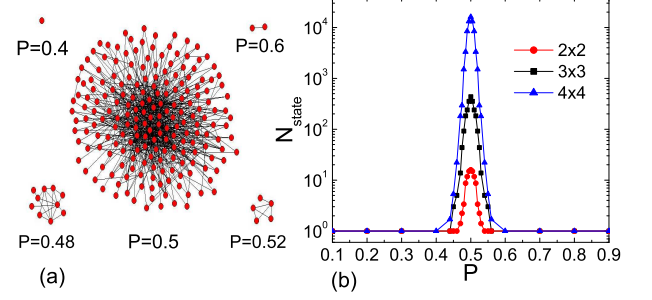


FIG. 5: (a) Prototypical examples of coarse-grained state networks for different biased parameter P . The simulations only last for 500 time steps for clear vision. (b) The number of states in the shrunk state networks by using 2×2 , 3×3 and 4×4 boxes, respectively. A sharp decline of the state number for different coarse-graining degree can be observed, which implies a phase transition from chaotic regime to ordered one.

state based on its randomly chosen Boolean function from 64 different functions (we fix the set of randomly chosen Boolean functions in the course of the time development. This model is usually called quenched model). After the updating procedure is finished at each time step, we perform the coarse-graining procedure and record a state $S(t)$ of the Boolean network together with a node to denote the state in the state space. Repeating above procedures for very long time steps, a weighted network is established. Surprisingly, in the case of using 4×4 boxes, the coarse-grained network shows perfect power-law distributions of in-strength and in-degree, out-strength and out-degree, as well as weight as shown in Fig. 2 to Fig. 4. The simulations last for 10^6 time steps. Each distribution is obtained with an average taken over 20 different SF network structures. These results indicate that the state graph in the chaotic regime near the edge of chaos is highly heterogenous with few states being reached from or going out to large amount of other states and most states being reached or going out for few times. Those highly connected nodes might be judged as attractors. However, these attractors fundamentally differ from the attractor cycles existing in the ordered regime. When the state trajectory falls into an attractor cycle, the complex dynamics will determinately evolve along this cycle forever [4]. While for the so-called attractors, although the trajectory falls into an attractor, it still can go out from the attractor. The distribution of weight also exhibits a power law, which implies the system evolves from some specific states to others with high probability. All the five power-law distributions demonstrate the SF Boolean network experiences a nontrivial self-organized process in the chaotic regime near the edge of chaos.

In order to prove that the observed power-law behaviors are not the artifact of the coarse-graining, we further

investigate more heavily coarse-grained state networks by using 3×3 boxes with $N = 99 \times 99$ Boolean nodes, as shown in the insets of Fig. 2 to Fig. 4. It is found that the distributions of strength and weight display the same power-law distributions in the case of adopting 4×4 boxes. However, the degree distributions show the exponential cut off for large degree nodes, which is attributed to finite size of the state space (for 3×3 boxes, the state space is composed of $2^{3 \times 3} = 512$ different states). While the power-law distributions of strength and weight are not influenced by the finite size effect. Moreover, it is worthwhile to emphasize that all the coarse-grained boxes contain the same number of Boolean variables, thus each coarse-grained state node contains the same number of state nodes in the original state. Suppose that if the original state network is a random network, then the coarse-grained one must be also a random network. Overall, we can conclude that the power-law distributions of the coarse-grained state network is expected to be the genuine property of the SF Boolean networks, not the artifact of the coarse-grained information.

To give further evidence for supporting above statement, we investigate the number of state nodes in the coarse-grained state network as a function of the biased parameter P , as shown in Fig. 5. One can find that different state nodes for $P = 0.5$ are so many that they nearly fill in the entire coarse-grained state space. While when the value of P departs from 0.5, there is a sharp decline of the number of states, as shown in Fig. 5 (b). This remarkable change demonstrates a phase transition from chaotic regime to ordered one. In the cases of P far from 0.5, there exists exclusive one node which is the shrunk attractor cycle in the ordered regime. Therefore, the behaviors of the SF Boolean network can also be reflected by the coarse-grained state networks. Fig. 5 (a) shows some examples of state networks for different value of P . The network with $P = 0.5$ possesses typical scale-free features that a few nodes (in the center) have large amount of connections while most nodes have a few links. When P is slightly larger or lower than 0.5, few state nodes exist.

We also study the Derrida curve [11] in the case of $P = 0.5$, as exhibited in Fig. 6. The Derrida curve has a nonzero intersection point with the line of slope 1. This critical crossover point (a stable fixed point) demonstrates the system is indeed in the chaotic regime, as we have mentioned early.

In conclusion, we have investigated the dynamics of large scale-free Boolean networks. By adopting the coarse-graining procedure performed in the state space, we find the state networks near the edge of chaos in the chaotic state exhibit perfect power-law distributions of in and out strength, in and out degree as well as weight. The simulations for different coarse-graining level and different evolutionary time, as well as different biased parameter demonstrate that the observed universal power-law

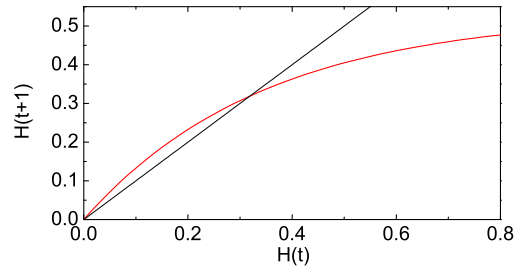


FIG. 6: Fitted Derrida curve of the original Boolean network for $P = 0.5$. The network size is $N = 100 \times 100$, $H(t)$ is the Hamming Distance at the time step t .

distributions are not the artifacts of coarse-graining procedure. Therefore, we can conclude that the SF Boolean networks in the chaotic state still perform well-defined self-organized behaviors.

Moreover, since much evidence has suggested that brain i.e. neural network is in a chaotic state [12] and has scale-free structural properties [13], our work in a certain extent may also be useful for characterizing and understanding the dynamics of brain, the complexity of which is beyond imagination. Although the state of each nerve cell can not be measured due to the experimental limitation, the dynamics of brain still could be reflected by the coarse-grained measurement.

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